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TITLE: MONTE CARLO SAMPLING STRATEGIES FOR LATTICE GAUGE CALCULATIONS

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MONTE CARLO SAMPLING STRATEGIES FOR LATTICE GAUGE CALCULATIONS

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We have sought to optimize the elements of the Monte Carlo processes for thermalizing and decorrelating sequences of lattice gauge configurations and for this purpose, to develop computational and theoretical diagnostics to compare alternative techniques. These have been applied to speed up generations of random matrices, compare heat bath and Metropolis stepping methods, and to study autocorrelations of sequences in terms of the classical moment problem.

The efficient use of statistically correlated lattice data is an optimization problem depending on the relation between computer times to generate lattice sequences of sufficiently small correlation and times to analyze them. We can solve this problem with the aid of a representation of auto-correlation data for various step lags as moments of positive definite distributions, using methods known for the moment problem to put bounds on statistical variances, in place of estimating the variances by too-lengthy computer runs.

MONTE CARLO SAMPLING STRATEGIES FOR LATTICE GAUGE CALCULATIONS

INTRODUCTION

We present here an overview of approach to statistical sampling and diagnostic techniques which we have found useful for lattice gauge calculations for elementary particle physics. The objective was to compute particle masses and other particle data in the quantum chromodynamic theory, with the four-dimensional space-time continum modeled as a discrete lattice. The dynamical method follows the Feynman path-integral formulation with the many-dimensional integrals done by Monte Carlo sampling. The method has been developed intensively in the last decade by many workers, and seems to be the most promising technique for quantitative success in the testing of fundamental theories of the strongly-interacting elementary particles.

Inevitably, this technique, or any other, will strain the memory and computing-speed capabilities of the most modern computers. The physicist's expertise must be supplemented by new categories of expertise, in numerical analysis, statistical analysis, and programming, and these latter subjects generate their own topics for research, one aspect of which is the concern of this paper.

We consider the thermalization and decorrelation of Markov sequences of calculated data, as generated by random stepping processes of the Metropolis type. While our context and numerical illustrations come from the lattice gauge problem, Monte Carlo methods for both classical and quantum statistical mechanics raise similar questions, and may have similar application.

FORMULATION

In broad outline, the formal structure we have to deal with is the following:

First, there is a "base set" consisting of a finite numer of elements. In our case, this is a four-dimensional lattice, with, typically, $12 \times 12 \times 12 \times 32$ or $20 \times 20 \times 20 \times 48$ sites. The latter size appears to be the maximum that can be reasonably explored on the Los Alamos CRAY X-MP.

Second, one seeks to construct an ensemble of configurations $\{x_0, x_1, x_2, \ldots\}$ each of which is a set of physical data associated with the base set. In the lattice gauge case, a configuration consists, in part, of an assignment of a 3×3 matrix to each of the links (lines between adjacent sites) on the lattice. The set of possible matrices A at each link comprises the group SU_3 and has the invariant measure $d\mu(A)$ of the group. Hence the configuration of matrices for the whole lattice has a measure which is the product of the measures for the links, and, because SU_3 is compact, the total measure is finite.

Third, the configurations in the ensemble should occur with a probability

$$p(x) \prod_{\text{links}} d\mu(A)$$

which is a kind of Bolzman weight factor defined by the theory.

Fourth, there is a family of functions $f(x)$ on the configurations, which represent measurements on them. The physical quantities to be calculated appear as averages,

$$\langle f \rangle = \int f(x)p(x)\Pi d\mu(A) \quad , \tag{1}$$

over the ensemble of configurations, and it is to those averages that the Monte Carlo sampling is applied.

Finally, the ensemble average (1) is replaced by an average $\bar{f}$ over a sequence $\{x_0, x_1, x_2 \ldots X_N\}$. The problem is then to generate sequences and deduce the statistical accuracy of the sequence averages, in order to (a) optimize the efficiency of the sequence generation, and (b) ascertain the statistical uncertainty in the results.

Consider a random sampling procedure for configurations in which $W(y,x)$ represents the probability that if a configuration x is at hand, then a configuration y will be chosen. If the total number of configurations were finite, and equal to n, then W would be an $n \times n$ matrix. This is not really the case, but it will be convenient to pursue our discussion in the framework of finite n for a while. Then $p(x)$ is taken as having n discrete values and

$$\sum_x p(x) = 1 \quad , \qquad \sum_y W(y,x) = 1 \quad .$$

Then a sequence $\{x_i\}$ may be constructed as follows:

(1) Choose x_0 arbitrarily. (Typically, all matrices A are taken as the identity matrix for x_0.)

(2) If the sequence has been chosen up to term x_i, and $x_i = y$, then choose configuration z with probability $W(z,y)$ and "accept" it, that is, set $x_{i+1} = z$, with probability $p(z)$. If it is not accepted, set $x_{i+1} = x_i$. Then the probability that $z = x_{i+1}$ follows $y = x_i$ is $F(z,y)$, where

$$F(z,y) = p(z)W(x,y) + \delta_{xy}(1 - \sum_{v} p(v)W(v,y)) \quad . \tag{2}$$

Then F satisfies

$$\sum_{z} F(z,y) = 1 \quad \text{and}$$

$$\sum_{y} F(z,y)p(y) = p(z) \quad ,$$

that is, F has eigenvalue 1 for vector $\underline{p} = \{p(z)\}$.

With suitable restrictions on W, one can now show that the sequence $\{x_i\}$ will be distributed with probability p(x). It is sufficient to suppose that W is symmetric and connected, i.e., some power of W connects each x and each y with non-zero probability. This procedure is a prototype of the so-called heat bath and Metropolis stepping mthods used to generate lattice gauge sequences. While there are a number of procedures which vary the form of the prescription, they amount to the same thing.

AUTOCORRELATIONS

When stochastic matrices like F and W are considered finite dimensional, they can be treated by elementary algebraic methods; their significant properties were first studied by Frobenius and Perron.[1] In particular

(1) F has a non-degenerate eigenvalue e of unity [corresponding, in our case, to the known eigenvector p(x)].

(2) All other eigenvalues e_i have $|e_i| < 1$.

(3) in the limit $m \to \infty$, F^m converges to a constant matrix F_∞ all of whose columns are equal to the eigenvector for e = 1.

Thus, if x_i, the $i^{\underline{th}}$ configuration of the sequence is y, the probability that z is the (i + m)th configuration is $F^m(z,y)$ and this is p(z), independent of x_i, for all sufficiently large m. This property is also independent of W, but the magnitude of the "sufficiently large m" will depend on choice of W.

The sequence is "thermalized" after m steps if the probabilities for x_i, $i \geq m$, are independent of the original choice x_0. The "transient" part of the sequence, with $i < m$ is ordinarily discarded before a sequence average is taken. For the remaining, thermalized portion of the sequence, the "decorrelation time" is the number of steps m such that the distribution of x_{i+j} is independent of x_i for $j \geq m$. (This means the distribution

approximates $\rho(z)$ to within an acceptably small error.) In lattice gauge problems thermalization and decorrelation times can vary from 5 or 10 to several hundred, depending on the problem and the wisdom of choice of W.

Let the sequence, after discarding of the transient phase, be $\{x_i\}$, $1 \leq i \leq N$. If the configurations were uncorrelated, the variance in a sequence average

$$\bar{f} = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \tag{3}$$

would be σ^2/N, with σ^2 estimated by the sample average

$$\sigma^2 = \frac{1}{N-1} \sum_{i=1}^{N} (f(x_i) - \bar{f})^2 \quad . \tag{4}$$

But in the case of correlation, σ^2 must be replaced[2] by an effective variance, σ^2_{eff}:

$$\sigma^2_{eff} = \sigma^2 \left[\rho_0 + 2 \sum_{i=1}^{N} (1 - \frac{i}{N}) \rho_i \right]$$

where ρ_k, the autocorrelation with lag k, is estimated from the sample by

$$\rho_k = \frac{\sum_{i=1}^{n-k} (f(x_i) - \bar{f})(f(x_{i+k}) - \bar{f})}{\sum_{i=1}^{N} (f(x_i) - \bar{f})^2} \quad . \tag{5}$$

This definition implies $\rho_0 = 1$, $|\rho_k| \leq 1$ for $k \geq 1$. The sequence would be "decorrelated after r steps" if ρ_k for $k \geq r$ is zero to within some acceptably small error. The sample estimate, Eq. (5) is subject to its own errors; more on this later. For $r \ll N$ (which we hereafter assume) the effective variance simplifies to

$$\sigma^2_{eff} = \sigma^2 \left(1 + 2 \sum_{i=1}^{r} \rho_i \right) \quad . \tag{6}$$

The relevance of the autocorrelations ρ_k follows from their connection with the effective variance σ^2_{eff} for $\bar{f}$. They depend, in part, on the sequence $\{x_i\}$ and in part, on the choice of measurement $f(x)$.

A practical concern can arise as follows:

Suppose an average $\bar{g}$ of a measurement $g(x)$ is sought where the computer time to get $g(x_i)$ is much larger than the time to get x_i from x_{i-1}. Suppose we expect that 100 uncorrelated values of $g(x)$ are enough to get $\bar{g}$

to desired accuracy. Should we then compute 1000 configurations and compute g(x) for every 10th, or compute 10,000 configurations and g(x) for every 100th, or do even more? As will be noted later, 100 values of g(x) may be wholly inadequate for an internal analysis of the statistical independence of these values. Also, if there are a variety of W's available, how do we access the most rapidly decorrelating one if the calculation of the g(x)'s is so lengthy? It would be convenient if a proxy measurement f(x), whose calculation time is short compared to the time to get x_i from x_{i-1}, could be relied on to get the decorrelation time for various candidate W matrices.

AUTOCORRELATIONS AS MOMENTS

We continue, for awhile, to regard W and F as finite dimensional matrices. The configurations are indexed by i, $1 \leq i \leq n$. The probability function is p_i, $1 \leq i \leq n$.

Let Z be the diagonal matrix whose (i,i) element is $\sqrt{p_i}$. Then by (2),

$$F = Z^2W + \text{diagonal matrix}$$

Hence

$$\begin{aligned} Z^{-1}FZ &= ZWZ + \text{diagonal matrix} \\ &= \text{symmetrix matrix} \\ &= UDU^{-1} \quad . \end{aligned}$$

U is some orthogonal matrix and D is real and diagonal with diagonal elements u_α, $1 \leq \alpha \leq n$. Then

$$F = (ZU)D(ZU)^{-1}$$

and

$$F^k = (ZU)D^k(ZU)^{-1}$$

are representations which will allow us to separate out the f(x)-dependent and W-dependent aspects of the autocorrelations ρ_k.

Consider the expression of ρ_k as a sequence average, Eq. (5), replaced by an ensemble average. The components of F are:

$$F_{jm} = \sum_\alpha (ZU)_{j\alpha} u_\alpha (ZU)^{-1}_{\alpha m} \quad .$$

Let $\alpha = 1$ represent the unit eigenvalue $u_1 = 1$; then U_{j1} is the column $\sqrt{p_j}$ and $(ZU)^{-1}_{j1}$ is the column p_j. The probability that x_i is the i^{th} configuration in the sequence, is configuration j is p_j, and the contingent probability that x_{i+k} is configuration m if x_i is j is $(F^k)_{jm}$. The ensemble average representation of the covariance sum is, for large N,

$$\frac{1}{N}\sum_{i=1}^{N-j}(f(x_i)-\bar{f})(f(x_{i+k})-\bar{f}) = \frac{1}{N}\sum f(x_i)f(x_{i+k}) - \bar{f}^2$$

$$\to \sum_j\left[f_j p_j \sum_m \left(F^k\right)_{jm} f_m\right] - \langle f\rangle^2$$

$$= \sum_\alpha \sum_j f_j \sqrt{p_j}\, U_{j\alpha}\ (u_\alpha)^k \sum_m f_m \sqrt{p_m}\, U_{k\alpha}$$

$$- \left(\Sigma f_i p_i\right)\left(\Sigma f_m p_m\right) = \sum_\alpha{}' C_\alpha(f)^2 (u_\alpha)^k$$

where

$$C_\alpha(f) = \sum_j f_j \cdot \sqrt{p_j}\, U_{j\alpha}$$

is a kind of projection coefficient of f(x) in the diagonal cordinate frame for F, and Σ'_α means a sum over all eigenvalues u_α <u>except</u> $u_\alpha = 1$. Also

$$\sigma^2 = \frac{1}{N}\sum_{i-1}(f(x_i)-\bar{f})^2 \to \sum_\alpha{}'[C_\alpha(f)]^2$$

Thus, we arrive at the desired representation,

$$\rho_k = \sum_\alpha{}' h_\alpha (u_\alpha)^k \tag{7}$$

where

$$h_\alpha = \frac{[C_\alpha(f)]^2}{\Sigma'_\alpha [C_\alpha(f)]^2}$$

obeys

$$0 \leq h_\alpha \leq 1, \quad \sum_\alpha{}' h_\alpha = 1 \quad .$$

The weights h_α depend on f(x) and its projection onto the diagonal basis for F; the u_α depend on F alone, and $|u_\alpha| < 1$ for all u_α in the sum. The "decorrelation time" is the smallest k such that the k^{th} power of the maximum u_α is sufficiely close to zero, according to some error allowance. The decorrelation time depends on F but not on f(x).

EXTENSION TO THE GENERAL CASE

So far, we have regarded W and F as finite-dimensional matrices. In fact, the configurations x form a continuous space with a measure equal to the product of the SU(3) invariant measures for all the lattice links. F and W are transformations on the configuration space, and by extension, are transformations on the Hilbert space of functions f(x) with scalar product

$$\langle f|g\rangle = \int f^*(x)g(x)\Pi d\mu(A) \quad .$$

We can write $Wf(x) = \int W(x,y)f(y)\Pi d\mu(A)$, with W(x,y) continuous and bounded. Because the underlying space is compact and its total measure is finite, W is a Hilbert-Schmidt operator, with the consequence that its eigenvalue spectrum, and hence the spectrum $\{u_\alpha\}$ of F, is discrete with a possible point of accumulation only at zero. The generalization of the Frobenius-Perron result of a unique eigenvector for eigenvalue unity, with other eigenvalues strictly less than unity in magnitude is also available.[3] Therefore, Eq. (7) remains valid, as an infinite sum, with only a finite number of eigenvalues outside a neighborhood of zero.

The k^{th} autocorrelation now appears as the k^{th} moment of a discrete distribution $d\sigma$ limited to the interval (-1,1). We believe that for our sampling procedures, the interval is always in (0,1); (i.e., there are no "anticorrelations") but have not been able to prove it; this is probably a simple oversight on our part.

If the first 2m moments, i.e. $(\rho_0 = 1, \rho_1, \ldots \rho_{2m-1})$ of $d\sigma$ are known, then the gauss quadrature procedure allows, by standard methods, the calculation of m weights (approximate k_i) and m nodes (estimates for the eigenvalues) such that

$$\int g(\alpha)\, d\sigma \cong \sum_{i=1}^{m} h_i\, g(u_i) \quad ,$$

with the approximation exact for g(x) a polynomial of degree $\leq 2m-1$.
The eigenvalue estimates will tend to be more accurate for the largest eigenvalues, which is what we want in order to estimate decorrelation rates. On the other hand, the calculations of nodes from moments can be sensitive to rather small errors, including statistical errors in the moments, and in our study, were very sensitive. Bartlett[4] has given an approximation to the variance of a sample estimate for autocorrelations based on assumption of a multinormal parent distribution; he finds

$$\mathrm{var}(\rho_k) \sim \frac{1}{N}[\sigma^2 + 2\Sigma_j(\rho_j)^2] \qquad (8)$$

for large k, i.e., var (ρ_k) accumulates with the correlations themselves, and the noise level for large or even moderate k can disrupt a calculation of gauss data and obscure the assessment of a correlation time from the list of ρ_k. In our lattice gauge experiments, N = 1000 was generally an insufficient length for a sequence, and N = 10,000 often barely sufficient.

SOME APPLICATIONS

Autocorrelations on averages over plaquette traces (traces of the product of a sequence of link matrices along a closed, rectangular path of links) were done on our 12 × 12 × 12 × 32 lattice calculation of particle masses, for plaquettes from 1 × 1 up to 6 × 6. These indicated decorrelation after 30-50 steps, but error estimates on our method were less refined at the time, and we may have judged too conservatively.

On a more systematic basis, we analyzed, on a 3 × 3 × 3 × 6 lattice, decorrelation of the 1 × 1 plaquette trace average, over a wide variety of sequence-generating algorithms of the Metropolis and heat bath types. The algorithm already proposed[5] for trace-biased random selection of stepping matrices held up very well, on a comparative basis, and we believe that ρ_1 for the 1 × 1 plaquettes, or at least the first 2 or 3 ρ's serve well as a diagnostic to discriminate among candidate algorithms. Over a range of β parameters from 5 to 7, the referenced method was insensitive to the choice of average trace for the random stepping matrix; anything from 2.6 to 2.8 gave nearly optimum decorrelation rate. In terms of net computer time, a hit rate of about 20 was cost-effective over higher rates, although 50-60 hits were needed to saturate the heat-bath limit. The latter, in turn seemed more cost-effective than the Pieterinen heat-bath. A discussion of the Cabibbo-Marinari approach will be given elsewhere. Because of the noise in statistics, there were (infrequent) inconsistencies in the apparent predictions even for 10,000 step sequences, which could be rectified by comparing several autocorrelations, or by looking at a 20,000 run in suspicious cases.

We sought to estimate the eigenvalues for a 20-hit algorithm on a 6 × 6 × 6 × 6 lattice and also the weights for plaquette averages, of sizes 1 × 1 to 3 × 3 and for certain quantitites E_i, B_i (gauge analogues of electric and magnetic fields) relevant to predicting glueball masses. Again, a run of 10,000 configurations, taking 5.8 hours of CRAY-XMP computing time.

The magnitude of greatest interest is the maximum eigenvalue u_{max} as the inequality $\rho_k \leq (u_{max})^k$ gives a direct estimate of decorrelation rate. The simplest estimate is

$$u_{max} = \lim(m \to \infty)\ (\rho_m)^{1/m}$$

More generally. one can set

$$\rho_k = \sum_{i=1}^{m} h_i (u_i)^k \quad \text{for } 0 \leqq k \leqq 2m-1 \quad ,$$

corresponding to an $2m^{th}$ order gauss approximant to $d\sigma$. Alternatively, set

$$\rho_k = \sum_{i=0}^{m} h_i (u_i)^k \quad \text{for } 0 \leqq k \leqq 2m$$

with u_0 set at 0 (h_0 contributes only to a_0), which corresponds to a left Radau approximant of order $2m + 1$.

The first two recipes necessarily provide a sequence of underestimates of u_{max}, and one hopes to see the sequence saturating at some upper bound. But it proved difficult to make use of ρ_k's in the gauss or radau approaches for $k \geqq 4$ or 5 because of the noise in the statistics.

Table I shows how the $(\rho_m)^{1/m}$ estimate for u_{max} fares for 1×1, 2×2, 3×3 plaquette averages and an overall E-field + B-field average. Convergence for increasing m is offset by increasing percentage of noise for increasing m. The sequence of estimates must terminate when ρ_m is smaller than the standard deviation, which is about 0.015, as inferred from Eq. (8). A u_{max} in the neighborhood of 0.8 is indicated.

Potentially more accurate (except for the noise!) is Table II. The gauss (4) model, using the first four autocorrelaton data and supplying two nodes plus two weights suggests a u_{max} again in the neighborhood of 0.8, and a substantially smaller (hence less accurately estimated) node. The other models, which utilize higher autocorrelations do not add much to this picture. Thus, the gauss (6) model has a u of 4.10 and some negative u's, albeit with extremely small h's; these are theoretically not possible for a noiseless set of autocorrelations.

One disturbing feature is the suggestion of u_{max} of about 0.94 for the 3×3 plaquette for radau (7) (and also for gauss (8) and radau (9), not shown). Either this is a statistical fluctuation, or the data depending on long-distance correlations in the lattice may be coupled with a small, but not ignorable weight to a slowly decorrelating term not seen in the other columns because of much weaker coupling. A run of, say, 90,000 steps would reduce statistical error by a factor of three and settle this question, at a considerable cost in computer time.

The standard deviation of an estimated $\bar{f}$ from a sequence $\{x\}$ of N terms can be written

$$\text{stan. dev.} = \frac{\sigma}{\sqrt{N}} \gamma_{corr} \qquad (9)$$

where γ_{corr} is the addition factor due to autocorrelation. By Eq. (6), it can be bounded as follows:

$$1 \leq (\gamma_{corr})^2 \leq 1 + 2\,\Sigma\rho_k \leq 1 + 2\,\Sigma(u_{max})^2 \leq [(1 + u_{max})/(1 - u_{max})]^{1/2}$$

If, from a sequence of N terms, only every $n^{\underline{th}}$ configuration is retained for calculation of f(x), then the effective maximum eigenvalue is $(u_{max})^n$ and Eq. (9) is replaced by

$$\text{stan. dev.} = \frac{\sigma}{\sqrt{(N/n)}}\,\gamma_{corr}(n) \tag{10}$$

with

$$\gamma_{corr}(n) = \left(\frac{1 + (u_{max})^n}{1 - (u_{max})^n}\right)^{1/2} .$$

Illustrative values of $\gamma_{corr}(n)$ are tabulated in Table III. It is seen that if the estimate $u_{max} \sim 0.8$ is relied upon for our $6 \times 6 \times 6 \times 6$ lattice, very little is gained by taking $n > 10$ for the sequence averaging of a measurement f(x), even if the computation of f(x) is long compared to the computation of x_{i+1} from x_i.

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Table I. u_{max} estimated by $(\rho_m)^{1/m}$ for various lattice functions.

	1 × 1	2 × 2	3 × 3	E-field
m = 2	.595	.657	.631	.603
m = 4	.635	.709	.718	.679
m = 6	.648	.742	.767	.724
m = 8	.695	.772	.794	.759
m = 10	.752	.802	.825	.792
m = 12	.759	.808	.829	.800
m = 14	-	.789	.834	.786
m = 16	-	.801	.828	.799
m = 18	-	.812	.854	.815

Table II. Nodes and weights by various quadrature models for various lattice functions.

Model	1 × 1		2 × 2		3 × 3		E-field	
	u	h	u	h	u	h	u	h
gauss (4)	.26	.40	.07	.26	.05	.38	.13	.42
	.74	.60	.76	.74	.80	.62	.79	.58
radau (5)	0	.24	0	.16	0	.32	0	.50
	-.52	-.03	.27	.13	.73	.63	-.18	-.14
	.68	.79	.77	.71	1.18	.05	.76	.64
gauss (6)	(complex roots)		.06	.26	-.20	.09	-.6	-.0005
			.76	.74	.24	.38	.11	.40
			4.10	10^{-5}	.84	.52	.77	.60
radau (7)	(complex roots)		0	.23	0	.31	0	.35
			-.53	-.005	-2.12	.0007	-.45	-.02
			.74	.77	.64	.44	.73	.67
			1.32	.008	.94	.25	1.37	.006

Table III. Values of $\gamma_{corr}(n)$. [See Eq. (10)]

u_{max}	n = 5	n = 10	n = 15	n = 20	n = 25
.90	1.97	1.44	1.23	1.13	1.07
.80	1.40	1.11	1.04	1.01	1.00
.70	1.18	1.03	1.00	1.00	1.00
.60	1.08	1.01	1.00	1.00	1.00